UCLA College | Physical Sciences Chemistry & Biochemistry

Chem 218: Student Exit Seminar

Developing Highly Efficient Electronic Structure Theory Methods for Large Scale Simulations

By Wenfei Li
Prof. Neuhauser Group

Electronic structure simulations are now becoming an indispensable tool in chemistry research. The overall goal is to develop methods that give accurate results without sacrificing efficiency. In our group, we incorporate various computational techniques to drastically reduce the cost of simulations. This allows us to run large scale simulations that were not previously possible. Our major innovation is stochastic quantum chemistry, where we replaced the summation over thousands of deterministic orbitals to an average over much smaller number of stochastic orbitals, and sometimes only a few suffices. This leads to significant increase in efficiency. In this seminar, I will talk about my two projects under the stochastic quantum chemistry framework. The first project involved developing an embedding stochastic framework, where a sub-system of interest is treated using deterministic orbitals, while the rest of the system is treated using stochastic orbitals. This way, we can selectively reduce the stochastic errors associated with that sub-system. The second project involved finding an optimal DFT starting point for our stochasticGW code. Apart from that, I will also introduce our orthogonal projector augmented wave package. Compared with the norm-conserving pseudopotential approach, the PAW method will allow a lower kinetic energy cutoff, hence greatly enhances the efficiency of electronic structure theory simulations.

Wednesday, March 10, 2021
12:00 p.m.
Via Zoom

For questions, please contact: jzabala@chem.ucla.edu